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LOW TEMPERATURE TRANSPORT THROUGH A QUANTUM DOT: THE ANDERSON MODEL OUT OF EQUILIBRIUM

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The infinite-U Anderson model is applied to non-equilibrium transport through a quantum dot containing two spin levels weakly coupled to two leads. At low temperatures, the Kondo peak in the equilibrium density of states is split upon the application of a voltage bias. The split peaks, one at the chemical potential of each lead, are suppressed by non-equilibrium dissipation. In a magnetic field, the Kondo peaks shift away from the chemical potentials by the Zeeman energy, leading to an observable peak in the differential conductance when the non-equilibrium bias equals the Zeeman energy.

Low Temperature Transport through a Quantum Dot: The Anderson Model out of Equilibrium

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The behavior of an atomic impurity coupled to conduction electrons has become one of the paradigms of condensed matter physics. Competition between on-site Coulomb interaction and band hybridization produces the Kondo effect: a crossover from weak to strong coupling between the localized and band electrons below the Kondo temperature, T_K. The study of the Kondo effect has been limited, however, by the nature of the impurity system. Since it is a daunting task to drive the host metal out of equilibrium, it is the *equilibrium* properties of Kondo impurities that have been explored.[1]

In this paper we address a new Kondo system in which *non-equilibrium* is routinely achieved, namely a semiconductor quantum dot weakly coupled to its leads. It is already evident that Anderson's model[2] for a Kondo impurity - discrete, interacting levels coupled to a band - also describes quantum dots. Experimentally, the discrete spectrum of a single dot has been probed by transport[3–5] and capacitance[6] spectroscopy, while the strong on-site Coulomb interaction is observed in Coulomb-blockade conductance oscillations.[4,5,7] Theoretically, Anderson's model has provided an excellent description of these experiments both in equilibrium,[8,9] and non-equilibrium.[10] However, it is only the high temperature regime that has been explored experimentally, while it is below T_K that the Kondo effect emerges.

Since the Anderson Hamiltonian describes the quantum dot, at low temperatures

the dot must behave as a Kondo impurity. In fact, Glazman & Raikh[11] and Ng & Lee[12] have argued that at zero-temperature equilibrium the Kondo resonance in the density of states of spin-degenerate levels will always lead to perfect transparency of the quantum dot at the Fermi energy. In contrast, above the Kondo temperature, resonant tunneling occurs only at a discrete set of Fermi energies. Thus the Kondo effect will have a striking experimental signature in low-temperature transport through a quantum dot. Furthermore, in the quantum dot system the leads coupled to the dot are easily biased to non-equilibrium and the dot potential can be swept continuously with a gate. Thus new physical questions which were not relevant to magnetic impurities can be raised. In particular, what happens to the Kondo effect out of equilibrium ?[13] Since transport measurements on single quantum dots require significant applied bias, this question is of immediate importance.

In this Letter we combine several approaches (non-crossing approximation,[14] equations of motion,[15] perturbation theory, variational wavefunction calculation[16]) to present a consistent picture of low-temperature, non-equilibrium transport through a quantum dot. For spin-degenerate levels at equilibrium, the Kondo peak[17] in the density of states at the chemical potential (Fig. 1a) leads to resonant transmission through the dot.[11,12] A voltage bias between the left and right leads causes the Kondo peak to split, leaving a peak in the density of states at the chemical po-

tential of each lead (Fig. 1b). We find that the amplitudes of the split Kondo peaks are suppressed by a finite non-equilibrium lifetime. This lifetime results from dissipative transitions in which electrons are transferred from the high chemical potential lead to the low chemical potential one. As the voltage bias is increased, the lifetime decreases, resulting in a suppression of the Kondo peaks and thus a suppression of the differential conductance (Fig. 2a).[13] Upon application of a magnetic field, the Kondo peaks shift away from the chemical potentials by the Zeeman splitting, but in opposite directions for each spin (Figs. 1c and 1d). Interestingly, therefore, when the chemical potential splitting equals the Zeeman splitting, a Kondo peak shifted away from one chemical potential crosses the other chemical potential. We predict an observable peak in the differential conductance at this crossing[18] (Fig. 2b).

We model the quantum dot and its leads by the Anderson Hamiltonian[2]

$$H = \sum_{\sigma;k\in L,R} \epsilon_{k\sigma} c^{+}_{k\sigma} c_{k\sigma} + \sum_{\sigma} \epsilon_{\sigma} c^{+}_{\sigma} c_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{\sigma;k\in L,R} (V_{k\sigma} c^{+}_{k\sigma} c_{\sigma} + h.c.), \qquad (1)$$

where $c^{+}_{k\sigma}(c_{k\sigma})$ creates (destroys) an electron with momentum k and spin σ in one of the two leads, and $c^{+}_{\sigma}(c_{\sigma})$ creates (destroys) a spin-σ electron on the quantum dot. Since we are interested in temperatures smaller than the orbital level spacing in the quantum dot, we consider only a single pair of levels on the dot with energies $\epsilon_{\uparrow} = \epsilon_0 + \Delta\epsilon/2$ and $\epsilon_{\downarrow} = \epsilon_0 - \Delta\epsilon/2$. The third term in (1) describes the Coulomb interaction

between the two localized spins which we take to forbid double occupancy[19] ($U \to \infty$), while the fourth term describes the hopping between the leads and the dot.

Our aim is to calculate the current through the dot, J, which for the case of proportionate couplings to the leads, $\Gamma^L_\sigma(\omega) = \lambda\Gamma^R_\sigma(\omega)$, where $\Gamma^{L(R)}_\sigma(\omega) = 2\pi\sum_{k\in L(R)}|V_{k\sigma}|^2\,\delta(\omega - \epsilon_{k\sigma})$, can be expressed[20] in terms of the density of states, $-\frac{1}{\pi}\mathrm{Im}\,G^r_\sigma(\omega)$, as

$$J = \frac{e}{\hbar}\sum_\sigma \int d\omega\,[f_L(\omega) - f_R(\omega)]\;\Gamma_\sigma(\omega)\left[-\frac{1}{\pi}\mathrm{Im}\,G^r_\sigma(\omega)\right]. \qquad (2)$$

In Eq. (2), $\Gamma_\sigma(\omega) = \Gamma^L_\sigma(\omega)\Gamma^R_\sigma(\omega)/\,[\Gamma^L_\sigma(\omega) + \Gamma^R_\sigma(\omega)]$, and $G^r_\sigma(\omega)$ is the Fourier transform of the retarded Green function, $G^r_\sigma(t) = -i\Theta(t)\langle\{\mathrm{c}_\sigma(t), \mathrm{c}^\dagger_\sigma(0)\}\rangle$.

In order to calculate the Green function $G^r_\sigma(\omega)$ we use both the non-crossing approximation[14] and an equations-of-motion method.[15,8] The non-crossing approximation is based on an exact mapping of the infinite-U Anderson Hamiltonian (1) onto a slave-boson Hamiltonian. If vertex corrections are neglected, the propagators for the boson and the fermion degrees of freedom, which correspond, respectively, to the propagators for the empty site and a singly occupied site, obey a set of coupled integral equations. Numerical solution of these equations has been very useful in obtaining quantitative results for the equilibrium system,[14] including the occupations of the two spin-states in the presence of a magnetic field.[21] In this work we have

generalized the non-crossing approximation to non-equilibrium to produce densities of states, occupations, and the nonlinear current (2). However, as a large spin-degeneracy (large N) technique, the non-crossing approximation produces a Kondo peak even for the non-interacting system ($N = 1$). Consequently, for $N = 2$ in a magnetic field, it give rise to spurious peaks in the density of states at the chemical potentials.[22] Therefore, an equations-of-motion method was employed to complement the non-crossing approximation and isolate its shortcomings. This method corresponds to a resummation of low-order hopping processes and cannot produce a quantitative description of the Kondo effect. Nevertheless, this method is known[15] to give the right qualitative behavior at low temperatures. More importantly in the present context, since the equations-of-motion method is exact for $N = 1$, it gives rise only to the proper Kondo peaks (as identified by perturbation theory[22]).

The equations-of-motion method consists of differentiating the Green function $G^r_\sigma(t)$ with respect to time, thereby generating higher-order Green functions which eventually have to be approximated to close the equation for $G^r_\sigma(t)$. The procedure we employ here is the same as the one used in Ref. 8, which in the infinite-U limit leads to

$$G^r_\sigma(\omega) = \frac{1 - \langle n_{\bar{\sigma}} \rangle}{\omega - \epsilon_\sigma - \Sigma_{0\sigma}(\omega) - \Sigma_{1\sigma}(\omega)}, \tag{3}$$

with

$$\Sigma_{0\sigma}(\omega) = \sum_{k\in L,R} \frac{|V_{k\sigma}|^2}{\omega - \epsilon_{k\sigma} + i\eta}, \tag{4}$$

and

$$\Sigma_{1\sigma}(\omega) = \sum_{k\in L,R} \frac{|V_{k\bar{\sigma}}|^2 f_{L/R}(\epsilon_{k\bar{\sigma}})}{\omega - \epsilon_\sigma + \epsilon_{\bar{\sigma}} - \epsilon_{k\bar{\sigma}} + i\hbar/2\tau_{\bar{\sigma}}}, \tag{5}$$

where $f_{L/R}(\epsilon)$ is the Fermi distribution in the left/right lead and $\tau_{\bar{\sigma}}$ is the intermediate-state lifetime. $G^r_\sigma(\omega)$ has an overall amplitude proportional to $1-\langle n_{\bar{\sigma}}\rangle$, where $\langle n_{\bar{\sigma}}\rangle$ is the occupation of the other spin-state. Quantitative calculation of the occupations is beyond the scope of the equations of motion in the present approximation scheme. Accordingly, we use the occupations resulting from the non-crossing approximation, which are known to be quantitatively reliable in equilibrium.[21]

Within the equations-of-motion scheme, the Kondo peak for spin σ results from the self-energy, $\Sigma_{1\sigma}(\omega)$, due to virtual intermediate states in which the site is occupied by an electron of opposite spin, $\bar{\sigma}$. The remaining self-energy, $\Sigma_{0\sigma}(\omega)$, is the exact self-energy for the non-interacting case. Because of the sharp Fermi surfaces at low temperature, $\mathrm{Re}\{\Sigma_{1\sigma}(\omega)\}$ grows logarithmically at $\omega = \mu_{L,R} \pm \Delta\epsilon$, giving rise to peaks in the density of states, $-\frac{1}{\pi}\mathrm{Im}\, G^r_\sigma(\omega)$, near those energies. The peaks for the high-lying spin (low-lying spin) appear near $\omega = \mu_{L,R} + \Delta\epsilon$ ($\omega = \mu_{L,R} - \Delta\epsilon$). At zero-field and zero-temperature equilibrium, the intermediate states giving rise

to $\Sigma_{i\sigma}(\omega)$ have an infinite lifetime, and the true peak in the density of states has an amplitude corresponding to the unitarity limit.[17] Once either a voltage bias or a magnetic field is applied these intermediate states acquire a finite lifetime, τ_σ, which cuts off the logarithmic divergence of $\mathrm{Re}\{\Sigma_{i\sigma}(\omega)\}$, resulting in a suppression of the peak amplitudes. The lifetime, τ_σ, of spin σ can be calculated using second-order perturbation theory, yielding

$$\frac{1}{\tau_\sigma} = \frac{1}{\hbar}\sum_A \Gamma_\sigma^A(\epsilon_\sigma)(1 - f_A(\epsilon_\sigma)) + \frac{1}{4\pi\hbar}\sum_{\substack{A,B=L,R \\ \sigma'}} \int_{-\infty}^{\infty} d\epsilon \left[\frac{1}{(\epsilon_\sigma - \epsilon + i\eta)^2} + \frac{1}{(\epsilon_\sigma - \epsilon - i\eta)^2}\right] \times \left[\Gamma_\sigma^A(\epsilon)\Gamma_{\sigma'}^B(\epsilon - \epsilon_\sigma + \epsilon_{\sigma'})(1 - f_A(\epsilon))\, f_B(\epsilon - \epsilon_\sigma + \epsilon_{\sigma'})\right]. \quad (6$$

For a deep level at zero temperature and for constant Γ this simplifies to

$$\frac{1}{\tau_\sigma} = \frac{1}{2\pi\hbar}\sum_{\substack{A,B=L,R \\ \sigma'}} \Gamma_\sigma^A\,\Gamma_{\sigma'}^B\,\Theta(\mu_B - \mu_A + \epsilon_\sigma - \epsilon_{\sigma'})\frac{\mu_B - \mu_A + \epsilon_\sigma - \epsilon_{\sigma'}}{(\mu_A - \epsilon_\sigma)(\mu_B - \epsilon_{\sigma'})}, \quad (7)$$

which explicitly shows that the lifetime is non-zero only for finite bias or finite magnetic field.

In Fig. 1, we plot the density of states for two spins symmetrically coupled to two leads, consisting of Lorentzian bands of width $2W$, so that $\Gamma_\sigma^L(\omega) = \Gamma_\sigma^R(\omega) = \Gamma W^2/2(\omega^2 + W^2)$, with $\Gamma \equiv 1$ and $W = 100$. Results are shown for the non-crossing approximation (dashed lines), which is reliable for zero magnetic field, and for the

equations-of-motion method (continuous lines), which has the correct Kondo peak energies for all magnetic fields. In equilibrium and zero magnetic field, the density of states exhibits a single peak at the Fermi level as expected[17] (Fig. 1a). As the chemical potentials split, the Kondo peak also splits, giving rise to a suppressed Kondo peak at each chemical potential (Fig. 1b). Upon the application of a magnetic field, the densities of states for the two spins become different and the Kondo peaks shift away from the chemical potentials by the Zeeman splitting ($\Delta\epsilon = 0.2$ in Figs. 1c and 1d). The peaks move up in energy for the high-lying spin (Fig. 1c) and down in energy for the low-lying one (Fig. 1d).

The main conclusion of Fig. 1 is the emergence of new energy scales, not present in equilibrium. The Kondo peak in the equilibrium density of states splits out of equilibrium to two peaks spaced by the chemical potential difference $\Delta\mu$, and suppressed from equilibrium by the finite dissipative lifetime τ_σ. In Fig. 1(b), the lifetime broadening, $\hbar/\tau_\sigma$, is about the same as the temperature. It is apparent, however, from Figs. 1 (c) and (d), that neither the non-crossing approximation nor the equations of motion quantitatively determine the Kondo peaks at finite magnetic field. For this case we use the equations-of-motion result since it provides a good estimate of the Kondo peak positions (by comparison with perturbation theory). To understand the shift of the Kondo peaks with magnetic field, it is helpful to

recall how the peaks in the density of states derive from the eigenstates of the system. At $T = 0$, $G^r_\sigma(t)$ involves transitions from the N-particle ground state to all possible $N+1$ or $N-1$ states. At $B = 0$ the correlated ground state has a finite amplitude to have an empty site, and thus $c^\dagger_\sigma$ (c_σ) can generate transitions from the N-particle ground state to the ground state with one more (one less) electron. Since, by definition, the ground state energies differ by the chemical potential, the density of states includes a Kondo peak at the chemical potential. Within a variational calculation,[16] we find that at finite magnetic field the ground state is polarized, and adding or removing an electron produces no overlap with the new ground state. However, there is a correlated excited state of opposite polarization which can be reached, and which consequently gives rise to a peak in the density of states, shifted by the difference in energy between polarization states, *i.e.* the Zeeman energy.

The current follows immediately from the densities of states (2). In particular, the zero-temperature current is the integrated density of states between the two chemical potentials, weighted by the coupling to the leads $\Gamma_\sigma(\omega)$. At zero magnetic field, therefore, the Kondo peak at the Fermi energy gives rise to a linear-response conductance of $2e^2/h$ for symmetric barriers, corresponding to perfect resonant transmission through the quantum dot.[11,12] As the bias is increased the differential conductance falls rapidly (Fig. 2a).[13] This occurs firstly because the differential conductance due

to a peak in the density of states must fall off once $\Delta\mu$ exceeds the peak width, and secondly because the decreasing dissipative lifetime suppresses the peak amplitudes. Since the peaks in the density of states persist until the temperature is roughly one-tenth the coupling to the leads, Γ, the peak in the differential conductance is observable well above the Kondo temperature, T_K (Fig. 2a, continuous line).

In a finite magnetic field the Kondo peaks are shifted away from the chemical potential so they contribute very little to the conductance in linear response. As the bias is increased, however, the current carrying region between the chemical potentials grows, until at $\Delta\mu = \Delta\epsilon$, it reaches one Kondo peak in the density of states of each spin (see inset of Fig. 2b). In Fig. 2b, one therefore sees peaks in the differential conductance at $\Delta\mu = \Delta\epsilon$ (continuous line). In fact, by comparison with the non-crossing approximation (Fig. 1), we expect the equations of motion to underestimate the full strength of these peaks. Experimentally, observation of peaks in the differential conductance at $\Delta\mu = \Delta\epsilon$ would provide a "smoking gun" for the presence of Kondo pnysics in transport through a quantum dot.

In this work, we addressed the non-equilibrium behavior of Anderson's model for a magnetic impurity. Experimentally, the model describes low-temperature transport through a quantum dot, where non-equilibrium is readily accessible. We have shown that new energy scales emerge in non-equilibrium. Specifically, the difference in

chemical potentials $\Delta\mu$ and the inverse dissipation time $\hbar/\tau_\sigma$ lead, respectively, to splitting and suppression of the Kondo resonances in the density of states. Our results have led to a novel experimental prediction — when the Zeeman splitting of the spins, $\Delta\epsilon$, equals the applied bias, $\Delta\mu$, there will be a peak in the differential conductance, provided these energies are smaller than the coupling to the leads, Γ, and smaller than the depth of the levels, $\mu_{L,R} - \epsilon_\sigma$. Importantly, this signature of the Kondo effect persists, for a wide range of parameters, to temperatures $\sim \Gamma/20$, which may be magnitudes larger than the Kondo temperature. We hope that this work will encourage further efforts, both experimental and theoretical, to probe the non-equilibrium physics of interacting quantum systems.

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Figure Captions:

(1) Density of states for an Anderson impurity symmetrically coupled to two leads with chemical potentials μ_L and $\mu_R(=0)$ and Lorentzian bandwidth $2W$, from the equations-of-motion method (continuous line) and the non-crossing approximation (dashed line). The impurity has two spin states with energies $\epsilon_\uparrow$ and $\epsilon_\downarrow$ and an on-site interaction $U \rightarrow \infty$. All energies are in units of the total coupling to the leads, Γ. The band width is $W = 100$ and the temperature is $T = 0.005$, roughly a factor of two lower than the magnetization Kondo temperature [Ref. 14]. (a) The equilibrium ($\mu_L = 0$) density of states at zero magnetic field $\epsilon_\uparrow = \epsilon_\downarrow = -2.0$. The density of states exhibits a single peak at the Fermi level [Ref. 17]. (b) The non-equilibrium ($\mu_L = 0.3$) density of states at zero magnetic field $\epsilon_\uparrow = \epsilon_\downarrow = -2.0$. There is a suppressed Kondo peak at each chemical potential. (c),(d) The non-equilibrium ($\mu_L = 0.3$) density of states for spin up (c) and spin down (d) at finite magnetic field $\epsilon_\uparrow = -1.9, \epsilon_\downarrow = -2.1$. The Kondo peaks shift away from the chemical potentials by the Zeeman splitting $\Delta\epsilon = 0.2$; the shift is up in energy for the up spin and down in energy for the down spin.

(2) Differential conductance, $e\,dJ/d\Delta\mu$, with $\mu_R = 0$, vs. applied bias. (a) Zero magnetic field differential conductance via the non-crossing approximation. (b) Differential conductance at the finite magnetic field, $\Delta\epsilon = 0.2$, used in Figs. 1 (c) and

(d), via equations of motion. As shown in the inset, when the chemical potential difference, $\Delta\mu$, reaches the Zeeman splitting, $\Delta\epsilon$, the Kondo peaks in the density of states enter the region between the chemical potentials, giving rise to a peak in the differential conductance.

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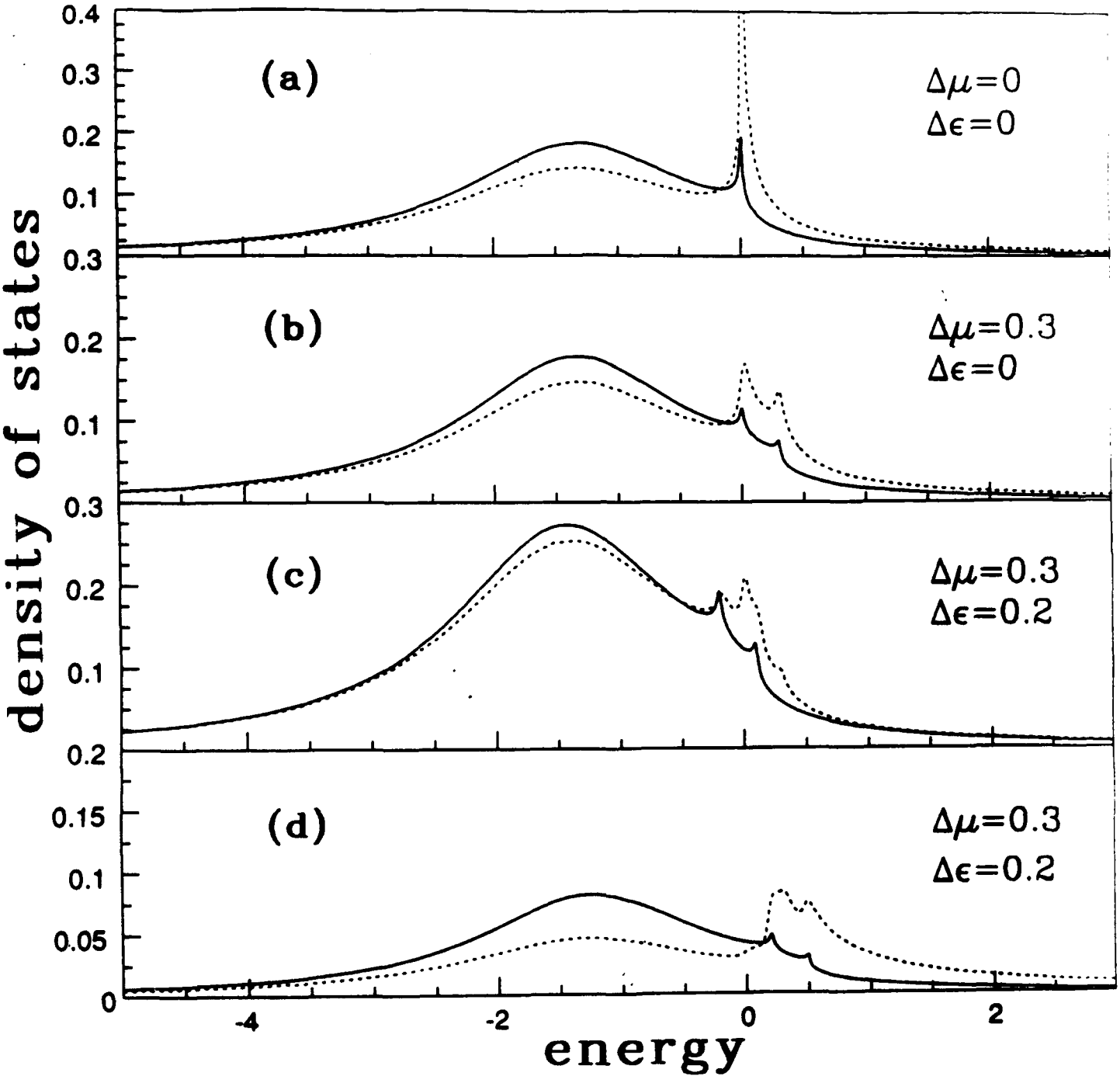
density of states
energy
(a)
Δμ=0
Δε=0
(b)
Δμ=0.3
Δε=0
(c)
Δμ=0.3
Δε=0.2
(d)
Δμ=0.3
Δε=0.2
0.4
0.3
0.2
0.1
0.3
0.2
0.1
0.3
0.2
0.1
0.2
0.15
0.1
0.05
0
-4
-2
0
2

Fig 1

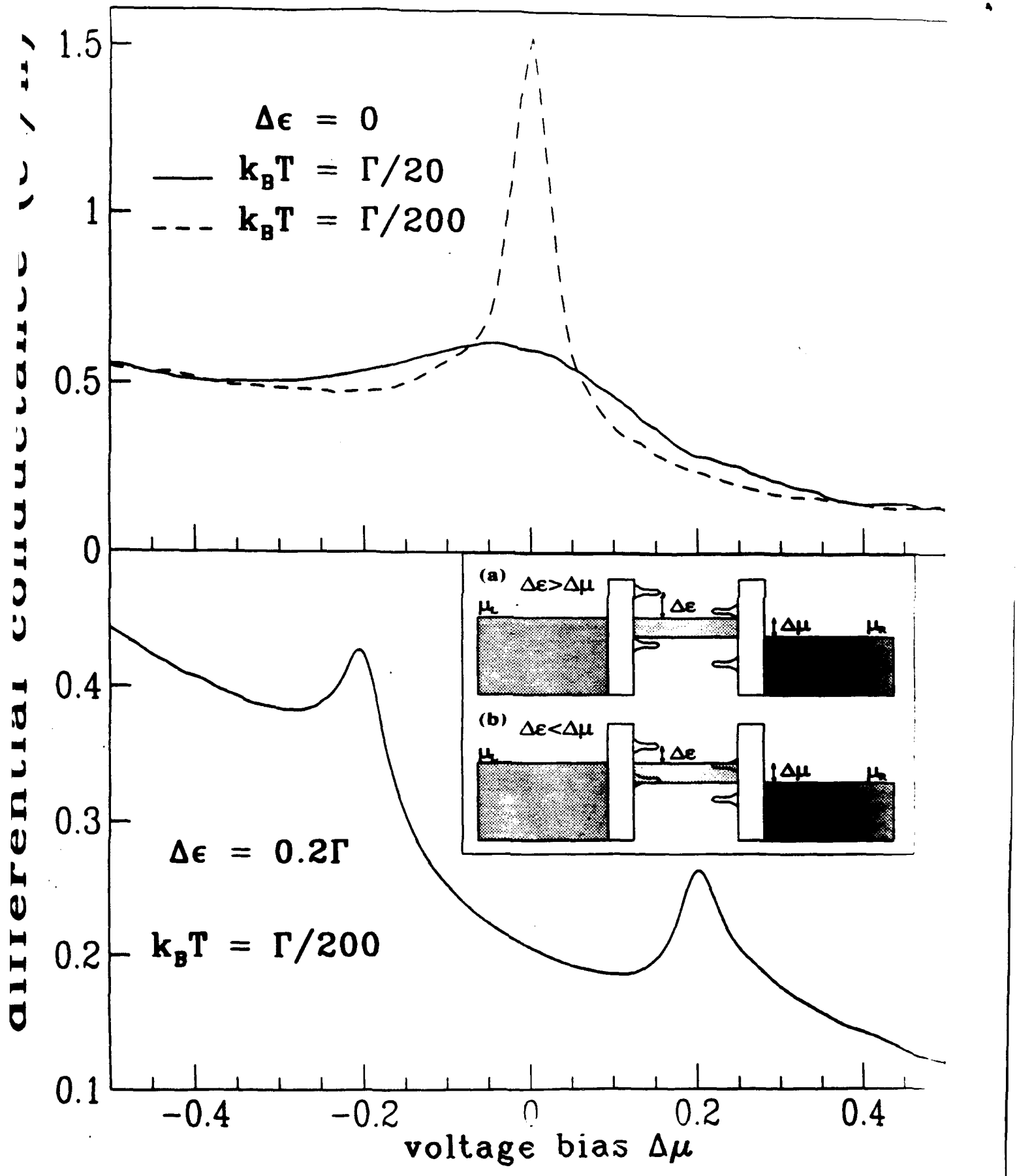
differential conductance
1.5
1
0.5
0
Δε = 0
k_BT = Γ/20
k_BT = Γ/200
(a) Δε>Δμ
μ_L
Δε
Δμ
μ_R
(b) Δε<Δμ
μ_L
Δε
Δμ
μ_R
0.4
0.3
0.2
0.1
Δε = 0.2Γ
k_BT = Γ/200
−0.4
−0.2
0
0.2
0.4
voltage bias Δμ

Fig 2